8.1 MOLECULAR DYNAMICS OF CASCADES OVERLAP IN TUNGSTEN WITH 20-keV PRIMARY KNOCK-ON ATOMS - W. Setyawan, G. Nandipati, K. J. Roche, R.J. Kurtz (Pacific Northwest National Laboratory[1]); B. D. Wirth (University of Tennessee)

OBJECTIVE

The objective of this research is to investigate how existing vacancies and interstitial atoms influence the defect production of the next cascade and vice versa.

SUMMARY

Molecular dynamics simulations are performed to investigate the mutual influence of two subsequent cascades in tungsten. The influence is studied using 20-keV primary knock-on atoms, to induce one cascade after another separated by 15 ps, in a lattice temperature of 1025 K (i.e. 0.25 of the melting temperature of the interatomic potential). The center of mass of the vacancies at the peak damage during the cascade is taken as the location of the cascade. The distance between this location to that of the next cascade is taken as the overlap parameter. Empirical fits describing the number of surviving vacancies and interstitial atoms as a function of overlap are presented.

PROGRESS AND STATUS

Introduction

Displacement cascade damage accumulation simulations are typically performed with object kinetic Monte Carlo (OKMC) method in which surviving defects (cascade debris) obtained from molecular dynamics (MD) are added into the simulation domain. This methodology assumes that existing defects do not affect the collision process of the next cascade. If the overlap process is ignored, introducing the same cascade debris exactly on top of each other (perfect overlap) would result in doubling the size of the defect objects. However this is likely to be inaccurate in a real life because the existing vacancies may be completely erased by the next cascade's core during the peak damage. In this research, we investigate the effect of the overlap process on the number of defects.

Simulation Details

Molecular dynamics (MD) technique as implemented in LAMMPS [1] is employed to simulate displacement cascades. The interatomic potential developed by Juslin et al. [2] is used. An important feature of this potential for radiation damage is that it gives the correct order of stability among dumbbells: <111>, <110>, and <100> with the <111> configuration being the most stable.

From our previous experience of cascade simulation in tungsten, a 20-keV primary knock-on atom (PKA), without electronic loss, results in average 15.5 surviving Frenkel pairs, N_F = 15.5. This number is sufficient to produce observable overlap effect. Therefore, this energy is chosen for this study. A cubic box of side equals 64 lattice units (203.75 Å) is used with periodic boundaries in all axes. The total number of atoms is 524,288. The coordinate of the atoms is shifted by a vector = (0.1, 0.3, 0.5) Å. This shift effectively results in a velocity vector with high Miller indices for any atom directed towards the box's center. Before the displacement cascade, the system is equilibrated at 1025 K at zero pressure. Subsequently, for the cascade simulation, the volume is fixed and a border region as thick as two atomic layers is defined in all sides. A Nosé-Hoover thermostat at 1025 K with a time constant of 100 fs is applied to the border atoms to model heat extraction during cascade. The rest of the atoms are evolved within the microcanonical (*NVE)* ensemble. Every cascade is followed up to 15 ps.[1]

The center of mass of vacancies at the peak damage is taken as the location of the cascade. To estimate the distance between the initial position of the PKA to the cascade location, λ_{peak}, 25 separate simulations are performed. In these simulations, a PKA is chosen from near the center of the box and given a velocity with a random direction. We obtain an average of λ_{peak} = 34.3 Å. These simulations are then discarded.

[1] PNNL is operated for the U.S. Department of Energy by Battelle Memorial Institute under Contract DE-AC06-76RLO 1830.

For all cascades, a PKA will be chosen from a pool of atoms within a spherical shell of 34.3 $\pm$ 0.2 Å from the box's center, and given a velocity directed towards the box's center. There are approximately 367 atoms within such a shell.

Results

Two hundred cascades are generated which constitute the first set of the cascade, cascade-1. From this set, we obtain N_F = 15.4 $\pm$ 0.3, λ_{peak} = 35.7 $\pm$ 0.7 Å, and λ_{end} = 31.8 $\pm$ 0.7 Å (λ_{end} is the distance between the PKA's initial position to the center of mass of the surviving vacancies). Figure 1 shows the variation of λ_{peak} and λ_{end} among simulation runs. It is interesting to note that $\lambda_{end} < \lambda_{peak}$ as if there is a collective restoring momentum back towards where the PKA originates after the peak damage phase.

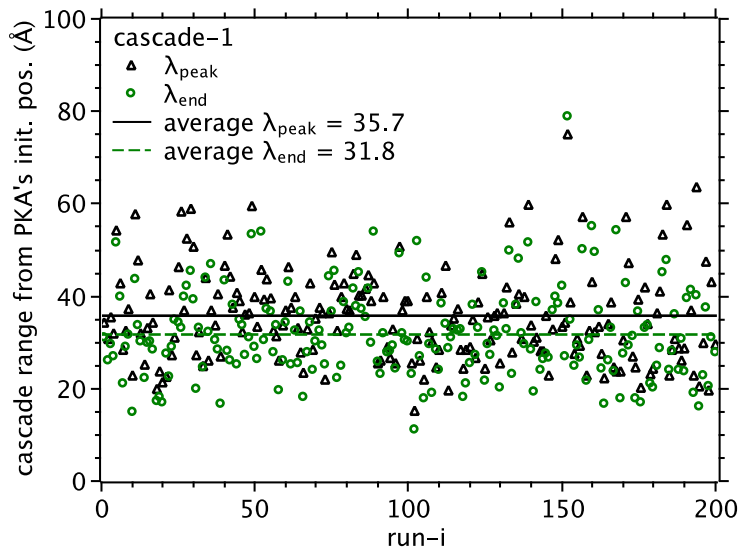

Figure 1. Variation of the distance from the PKA's initial position to the center of mass of vacancies at peak damage λ_{peak} (triangles) and to the center of mass of the surviving vacancies λ_{end} (circles) among simulation runs.

Cascades in cascade-1 are followed up to 15 ps. Afterwards, in each of these cascades, another PKA is chosen with the same procedure as described before to initiate a subsequent cascade. These subsequent cascades are again followed for 15 ps and constitute the second set of the cascades, cascade-2. The peak-to-peak damage distance between the first and the second cascade is taken as the overlap parameter, R_{pp}. Figure 2 shows the number of surviving vacancies at the end of cascade-2 as a function of R_{pp}. We fit the data to

$$N_{Vac,cascade-2} = N_\infty - \Delta \exp\left(-\left(R_{pp}/\alpha\right)^j\right)$$

where N_∞ is the number of vacancies when $R_{pp} = \infty$, therefore $N_\infty = 2 \times 15.4 = 30.8$. Parameters Δ and α are fitted for various integer values of j. The best fit is obtained with j = 2 and the fitted equation is

$$N_{Vac,cascade-2} = 30.8 - 10.6 \exp\left(-\left(R_{pp}/43.1\right)^2\right)$$

This result indicates that on average the net number of defects from the second cascade is smaller than the number of defects from the first cascade. At perfect overlap condition, the net value is (30.8-10.6)-15.4 = 4.8, i.e. the second cascade adds only 4.8 vacancies compared to 15.4 if the overlap process is ignored. We note that in 18 out of 200 runs, the net value is in fact < 0. Figure 2 also shows that the effect of the overlap is monotonic as a function of R_{pp}. This behavior will not be obtained in OKMC simulations which disregard the overlap process. In such OKMC simulations, most inter-cascade recombination

occurs at a certain overlap distance where the interstitials of the first cascade overlap with the vacancies of the second cascade and vice versa.

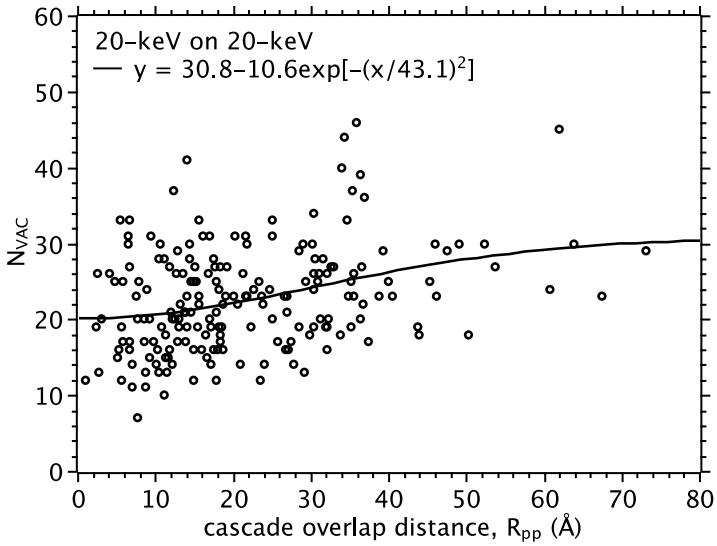

Figure 2. The number of surviving vacancies after the second cascade as a function of the distance between the center of mass of vacancies at the peak damage of the first and the second cascade, R_{pp}. The average number of surviving vacancies from the first cascades is 30.8/2 = 15.4.

If the time scale between subsequent cascades is much longer than that of SIAs diffusing away from the cascade region, practically only vacancies from the preceding cascade are left. To investigate the overlap effect for this situation, we construct another set of cascade overlap as follows. From run-1 to run-100 of cascade-1 set, another set is created by removing the existing SIAs and is denoted as cascade-1b. Cascade-2b is obtained after performing the second cascade on cascade-1b. The number of surviving vacancies and SIAs in cascade-2b is shown in Figure 3. The data points are fitted with a constraint of N_∞equals 30.8 and 15.4 for N_{Vac} and $N_{SIA,}$ respectively. The fit curves are

$$N_{Vac,cascade-2b} = 30.8 - 7.0\exp\left(-\left(R_{pp}/23.9\right)^2\right)$$
$$N_{SIA,cascade-2b} = 15.4 - 6.7\exp\left(-\left(R_{pp}/21.4\right)^2\right)$$

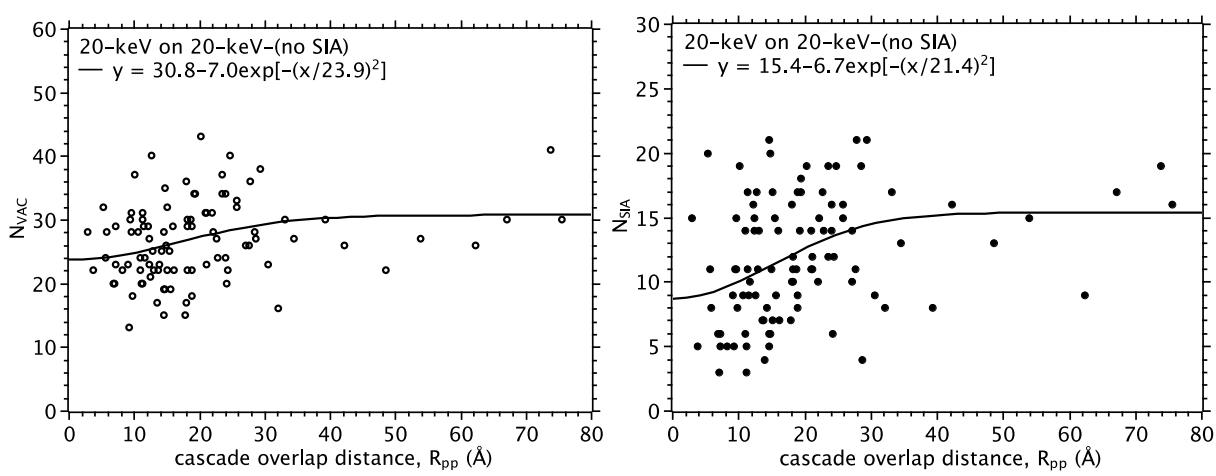

Figure 3. The number of surviving vacancies and SIAs after the second cascade with SIAs from the first cascade removed.

For a complete cascade overlap, the number of vacancies is 30.8-7.0. In other words, there is a reduction of 7 vacancies (or 7/30.8 = 23%) as compared to if a proper overlap simulation is not accounted for. Compared to cascade-2, the overlap effect in cascade-2b is smaller. In addition, the overlap region of influence parameter α is much shorter (23.9 Å) compared to that in cascade-2 (43.1 Å).

In the future, we will define another overlap parameter ϕ as follows. The vacancies from the first cascade are assigned type = 1 and are denoted as V_A. During the second cascade, any vacancies not occupying V_A are assigned type = 2 and denoted as V_B. If a V_A migrates during the second cascade to a location not occupied by any other V_A, then it becomes V_B. A V_A is flagged as overlapped if it has been a part of a V_AV_B cluster anytime during the second cascade. Consequently, a V_A that becomes a V_B will not be flagged as overlapped as long as it forms only a V_B cluster. The fraction of overlapped V_A to the initial number of V_A is taken as ϕ. Hence, ϕ has a value between 0 and 1 with 1 denoting a complete overlap. We will compare the merit as well as disadvantage between R_{pp} and ϕ as the overlap parameter.

References

[1] S. Plimpton, J. Comp. Phys. 117 (1995) 1.
[2] N. Juslin and B.D. Wirth, J. of Nuc. Mat. 432 (2013) 61.